# Phenomenological theory of spinor Bose-Einstein condensates

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It was reported that Bose-Einstein condensation induces a spontaneous magnetization in spinor bosons. This phenomenon is called Bose-Einstein ferromagnetism (BEF). We propose a phenomenological model consistent with the prediction of BEF and show that BEF might be attributed to the intrinsic magnetic moment of particles. Taking BEF into account, the phase diagram of an optically trapped spinor condensate is reexamined.

Alkali-metal atoms, such as $^{87}$Rb, $^{23}$Na, $^{7}$Li, in which Bose-Einstein condensation (BEC) has been experimentally realized[1], have an internal degree of freedom attributed to the hyperfine spin $F$. Accordingly, the order parameter of Bose condensed alkali atoms could have $2F+1$ components. Thus, although the superfluid properties of this system are considered to be essentially the same as those of superfluid $^{4}$He, one can expect that the hyperfine spin degrees of freedom could bring about remarkable differences between the two systems.

Earlier experiments leading to BEC in alkali atoms were performed in magnetic traps. A relatively strong external magnetic field $H$ was applied to confine the BEC system. Because the atomic spin direction adiabatically followed $H$, the spin degree of freedom was frozen. As a result, the alkali atoms behaved like scalar particles although they carried spin[2]. In 1998, Stamper-Kurn *et al.* succeeded in cooling $^{23}$Na in a purely optical trap and achieved BEC[3]. With $H$ sufficiently small, the spin degree of freedom can become active and the spinor nature of the condensate can be manifested[4].

The optical trap provides great opportunities to investigate spinor Bose gases experimentally. Furthermore, it stimulates enormous theoretical interest in studying various spin-related properties, e.g. the magnetism[5, 6, 7], of the gases. For an $F = 1$ Bose gas, the effective interactions $V(\mathbf{r})$ between the atoms were derived as[5, 6],

$$V(\mathbf{r}) = \frac{c_0}{2}\psi_\sigma^\dagger \psi_{\sigma'}^\dagger \psi_{\sigma'}\psi_\sigma + \frac{c_2}{2}\psi_\sigma^\dagger \psi_{\sigma'}^\dagger \mathbf{F}_{\sigma\gamma}\cdot\mathbf{F}_{\sigma'\gamma'}\psi_{\gamma'}\psi_\gamma \ , \ (1)$$

where $\psi_\sigma(\mathbf{r})$ is the field annihilation operator for an atom in hyperfine state $|F,\sigma\rangle$ ($\sigma = 1, 0, -1$) at position $\mathbf{r}$. Repeated sub-indices represent summation taken over all the hyperfine states. Besides a spin-independent scattering, a Heisenberg-like exchange interaction between hyperfine spins appears in the Hamiltonian, where the components of $\mathbf{F} = (F_x, F_y, F_z)$ are $3 \times 3$ spin matrices. According to the pioneering work of Ho[5] and Ohmi and Machida[6], this term determines the phase diagram of the spinor condensate: the ground state can be either ferromagnetic or "polar", depending on whether $c_2$ is negative or positive, respectively. However, recently Eisenberg and Lieb (referred to as EL hereafter)[8] claimed that this scenario ignored an intrinsic *ferromagnetism* of spinor bosons.

The intrinsic ferromagnetism in spin-1 ideal bosons was predicted by Yamada[9] and recently studied in the context of atomic Bose-Einstein condensation by Simkin and Cohen[10]. They calculated the magnetization $M(H)$ and found that once BEC takes place, $M$ remains finite even if $H = 0$, suggesting the system is magnetized spontaneously. This phenomenon is called Bose-Einstein ferromagnetism (BEF). Caramico D'Auria *et al.* pointed out that the coexistence of BEC with BEF also appears in *interacting* bosons[11]. Moreover, rigorous proofs presented by Sütő[12] and EL[8] show that a polarized state is among the degenerate ground state of spinor bosons. EL studied a Bose model with a *spin-independent*, totally symmetric interaction $v$ between particles,

$$H = -\sum_{i=1}^{N} \frac{\hbar^2}{2m}\nabla_i^2 + v(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N), \qquad (2)$$

where $\mathbf{r}_i$ denotes the spatial coordinate of particle $i$. The specific model of Caramico D'Auria *et al.* has the same symmetry as the above Hamiltonian.

In this communication, we propose a phenomenological model for the spinor Bose condensate. First of all, this model shows in a simple way that BEF can really take place at the same critical temperature as BEC. The results obtained are consistent with available theories. Then the phase diagram of optically trapped alkali atoms is reexamined, taking BEF into account. Furthermore, we try to understand the nature of BEF by analyzing the phenomenological model.

To begin with, we derive an appropriate Ginzburg-Landau free energy density functional for second-order phase transitions that describes the coexistence of BEC and BEF. Generally, such a free energy density consists of three different parts: $f_t = f_b + f_m + f_c$, corresponding to the Bose condensed phase, the ferromagnetic phase and the coupling between the two phases (we omit the free energy of the normal Bose gas). Following Ginzburg and Pitaevskii[13], the free energy density of an *isotropic*

spin-$F$ Bose-Einstein condensate is given as

$$f_b = \frac{\hbar^2}{2m}\nabla\boldsymbol{\Psi}^\dagger \cdot \nabla\boldsymbol{\Psi} - \alpha|\boldsymbol{\Psi}|^2 + \frac{\beta}{2}|\boldsymbol{\Psi}|^4$$
$$+\frac{\beta_s}{2}\Psi_\sigma^\dagger \Psi_{\sigma'}^\dagger \mathbf{F}_{\sigma\gamma} \cdot \mathbf{F}_{\sigma'\gamma'}\Psi_{\gamma'}\Psi_\gamma \ , \qquad (3)$$

where $\boldsymbol{\Psi}^\dagger \equiv (\boldsymbol{\Psi}^T)^* = (\Psi_F^*, \Psi_{F-1}^*, ..., \Psi_{-F}^*)$ is the complex order parameter and $|\boldsymbol{\Psi}|^2 = \boldsymbol{\Psi}^\dagger\boldsymbol{\Psi}$. Here the order parameter is defined as $\Psi_\sigma = \langle\psi_\sigma\rangle$, but we note that other forms of the order parameter are possible (see Leggett[2]). The free energy density should have the same symmetry as the underlying Hamiltonian. The first three terms describe a system without any spin-dependent interactions, as given by Eq. (2). The fourth term has SU(2) symmetry as does the $c_2$ term in Eq. (1), and describes the spin-exchange interaction.

The free energy density of the ferromagnetic phase can be expanded in powers of $M^2$: $f_m = aM^2/2 + bM^4/4$, where $M$ is the order parameter of the ferromagnetic state and is proportional to the magnetization density. In the usual theory of phase transitions, $a$ changes sign at the ferromagnetic transition temperature and $b > 0$[14]. Here, we assume that $M$ is induced by the BEC itself, rather than by any other additional mechanisms, so $f_m$ should have a minimum at $M = 0$. That is, the ferromagnetic state would disappear if it were not coupled to the Bose condensed state. Therefore, $f_m(M^2) \geq f_m(0) = 0$ for all values of $M$, so both $a$ and $b$ are *positive*. Near the critical temperature only the leading term need be considered, and $f_m$ takes the form,

$$f_m = \frac{a}{2}M^2 \ . \qquad (4)$$

Physically, $f_m$ should contain the energy of the magnetic field inside a magnetized medium[15]. We suppose that the condensate only couples linearly to the ferromagnetic order,

$$f_c = -gM\sum_{\sigma=-F}^{F}\sigma|\Psi_\sigma|^2 \ , \qquad (5)$$

where $g$ is the coupling constant. This is the simplest coupling term that satisfies the physical situation, as indicated later. Our discussions are confined to the thermodynamic limit and to one domain. Equations (4) and (5) comprise the basic ansatz of this work. We assume $a$ and $g$ are *independent* of the temperature.

The total free energy for the Bose condensate can be written as $F_T = \int f_t dV$. Taking the variation with respect to $\Psi_\sigma^*$, $\Psi_\sigma$ and $M$, we derive

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_\sigma - (\alpha + gM\sigma)\Psi_\sigma + \beta|\boldsymbol{\Psi}|^2\Psi_\sigma$$
$$+\beta_s\Psi_{\sigma'}^\dagger\mathbf{F}_{\sigma\gamma}\cdot\mathbf{F}_{\sigma'\gamma'}\Psi_{\gamma'}\Psi_\gamma = 0 \ , \qquad (6a)$$

$$aM - g\sum_{\sigma=-F}^{F}\sigma|\Psi_\sigma|^2 = 0 \ . \qquad (6b)$$

Eq. (6a) consists of a set of equations with respect to the spin index $\sigma$. Eq. (6b) ensures that the magnetization is induced by the condensate itself.

Possible phase transitions of the spinor Bose gas can be investigated by solving Eq. (6). For a spatially uniform system, the first term in Eq. (6a) can be dropped. We take the bosons to have spin $F = 1$. It has been suggested that the condensate should be ferromagnetic even *without the spin-exchange interaction*[8, 9, 10, 11]. To treat this case, we first set $\beta_s = 0$. Two nontrivial solutions deserve further discussion[16].

(I) *Normal Bose-Einstein condensates*. This solution corresponds to BEC without spontaneous magnetization.

$$|\boldsymbol{\Psi}|^2 = \frac{\alpha}{\beta} \ , \quad M = 0 \ , \qquad (7)$$

with the free energy density

$$f_t^I = -\frac{1}{2}\frac{\alpha^2}{\beta} \ . \qquad (8)$$

In this case, we have $|\Psi_1|^2 = |\Psi_{-1}|^2$ but cannot determine the proportion of $|\Psi_1|^2$ to $|\Psi_0|^2$. Thus, the system might be in "polar", "planar" or "equal spin" states[17].

(II) *Bose-Einstein ferromagnets*. This solution describes BEC with a spontaneous magnetization:

$$|\Psi_1|^2 = \frac{\alpha}{\beta - \frac{g^2}{a}} \ , \quad |\Psi_0|^2 = |\Psi_{-1}|^2 = 0 \ ,$$
$$M = \frac{g}{a}\frac{\alpha}{\beta - \frac{g^2}{a}} = \frac{g}{a}|\Psi_1|^2 \ . \qquad (9)$$

In this case the Bose condensate is fully polarized and the free energy density is

$$f_t^{II} = -\frac{1}{2}\frac{\alpha^2}{\beta - \frac{g^2}{a}} \ . \qquad (10)$$

Comparing Eqs. (10) and (8), it can be seen that the BEF solution is indeed energetically favored in spite of a positive magnetization energy $f_m$. The magnetization results in a net energy decrease by $f_t^I - f_t^{II} \approx g^2\alpha^2/(2a\beta^2)$[18], suggesting that $M \neq 0$ occurs *spontaneously*. This magnetization depends on the onset of BEC, with its magnitude proportional to the condensate density, as predicted in previous theories[9, 10, 11].

As usual[13], $\alpha$ can be expanded in powers of $T_c - T$ near the Bose condensation temperature $T_c$: $\alpha(T) \cong \alpha'(T_c - T)$; $\beta$ and $\alpha'$ are positive constants. According to Eq. (9),

$$M = \frac{g}{a}|\boldsymbol{\Psi}|^2 = \frac{g}{a}|\Psi_1|^2 \propto T_c - T \ . \qquad (11)$$

The results are consistent with those obtained from a microscopic interacting boson model[11], suggesting that the phenomenological model describes the behavior of the spinor condensates quite well.

The realization of BEC in optically trapped alkali-metal atoms makes the study on BEF not only theoretically interesting, but also experimentally attainable. We now turn our attention to such a specific BEC system. In this case, the $\beta_s$ term should be turned on. Using the notation $(\Psi_1, \Psi_0, \Psi_{-1}) = (\phi_1 e^{i\theta_1}, \phi_0, \phi_{-1} e^{i\theta_{-1}})$, the $\beta_s$ term becomes $\beta_s \phi_0^2 [\phi_1^2 + \phi_{-1}^2 + 2\phi_1 \phi_{-1} \cos(\theta_1 + \theta_{-1})] + \beta_s (\phi_1^2 - \phi_{-1}^2)^2 / 2$[19]. Without considering BEF, only this term determines the relative phases of the three component condensate wave functions: $\theta_1 + \theta_{-1} = \pi$ for $\beta_s > 0$ and $\theta_1 + \theta_{-1} = 0$ for $\beta_s < 0$. It therefore determines the ground state of the condensate: it is ferromagnetic for $\beta_s < 0$ and "polar" for $\beta_s > 0$[5]. However, this phase diagram is modified by BEF. After some algebra, the free energy density reduces to $f_t^P = -\alpha^2/(2\beta)$ for "polar" states and to $f_t^F = -\alpha^2/[2(\beta + \beta_s - g^2/a)]$ for ferromagnetic states. Consequently, the phase diagram illustrated in Fig. 1 results, with a phase boundary at a finite value of $\beta_s$, given by

$$(\beta_s)_c = \frac{g^2}{a} \ . \tag{12}$$

Equation (12) implies that there is a critical $\beta_s$ value leading to the "polar" state.

Strictly speaking, the Landau expansion holds mathematically only near $T_c$. In order to get the *ground state* phase diagram, we need decrease the temperature to zero, when the free energy density can be directly derived from the Hamiltonian via the Gross-Pitaevskii approximation. Because of the existence of BEF, we argue that *the energy due to the magnetization*, as expressed in Eqs. (4) and (5), should be included in the $T = 0$ free energy density functional. Then the Gross-Pitaevskii equation for the $F = 1$ bosons described by Eq. (1) reads:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_\sigma - (\mu + g^*M\sigma)\Psi_\sigma + c_0|\boldsymbol{\Psi}|^2\Psi_\sigma$$
$$+c_2\Psi_{\sigma'}^\dagger \mathbf{F}_{\sigma\gamma} \cdot \mathbf{F}_{\sigma'\gamma'}\Psi_{\gamma'}\Psi_\gamma = 0 \ , \tag{13a}$$

$$a^*M - g^* \sum_{\sigma=-F}^{F} \sigma|\Psi_\sigma|^2 = 0 \ . \tag{13b}$$

Here $\mu$ is the chemical potential. Equations (13) have similar forms as the phenomenological equations (6), but their parameters have *different* meanings[20], so here $a$ and $g$ are marked with a star. From Eq. (13), a phase diagram similar to Fig. 1 can be produced and the phase boundary becomes $(c_2)_c = (g^*)^2/a^*$ . The Gross-Pitaevskii approximation is quite accurate in describing the ground state of Bose gases.

We now discuss the origin of BEF. The possibility that BEF arises from an explicit spin-exchange interaction, like the $c_2$ term in Eq. (1), has been ruled out[8, 9, 10, 11]. Our phenomenological model shows clues that BEF may be attributed to intrinsic magnetic moments of particles. Since spinor bosons carry magnetic moments $\mathbf{m}$, an effective magnetic field $\mathbf{B} = \mu_0\mathbf{M}$
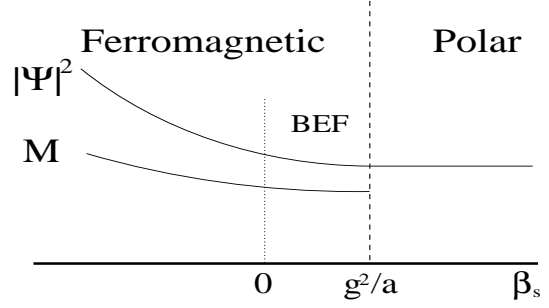


FIG. 1: Phase diagram of spin-1 Bose condensates. The schematic $\beta_s$-dependence of the two order parameters, $|\boldsymbol{\Psi}|^2$ and $M$, is outlined. Both decrease with increasing $\beta_s$ in the ferromagnetic state. At the phase boundary, $|\boldsymbol{\Psi}|^2$ is continuous but $M$ drops suddenly to zero, signaling a first-order phase transition. The intermediate region denotes the ferromagnetic state attributed purely to BEF.

is created inside a polarized body, owing to the superposition of the intrinsic field of all the magnetic moments. $\mu_0$ is the permeability of vacuum and $\mathbf{M} = \mathbf{m}|\Psi_1|^2$ is the magnetization. Naturally, $f_m = B^2/(2\mu_0) = \mu_0 M^2/2$ can be regarded as the energy of the effective field. On the other hand, the magnetic moment of the condensed bosons does respond to the magnetic field regardless if the field is external or internal, so the spin direction should follow the internal field $\mathbf{B}$. Eq. (5) just is the general form of the coupling between the condensate density and the internal magnetic field: $f_c = -\mu_0 mM|\Psi_1|^2 = -\mathbf{M} \cdot \mathbf{B} = -\mu_0 M^2$. Within this interpretation, $f_m + f_c = -\mu_0 M^2/2$, which is just the self-energy of a magnetized body with magnetization $\mathbf{M}$[15]. Contrarily, in the "polar" or "equal spin" states the magnetic moments of the particles are fully compensated: $M = 0$. Then at the mean-field level, an internal reference particle cannot sense the moments of other particles, and the magnetic self-energy is zero. Obviously the ferromagnetic state is energetically favorable at $T = 0$. At finite temperature, the ferromagnetic state can be destroyed due to an entropy increase. However, once Bose-Einstein condensation takes place, the temperature inside a condensate is absolutely zero and the ferromagnetic state remains stable. This accounts for the dependence of BEF on the onset of BEC. We note that such a interpretation coincides with the prediction of Yamada and Caramico D'Auria *et al.*, because in their calculations of magnetization at a given field, the magnetic moment of spinor bosons was included.

Simkin and Cohen attributed BEF to the Bose-Einstein statistics[10]. However, we notice that although the Bose-Einstein statistics does not exclude a ferromagnetic state in spinor bosons, it cannot lead to a spontaneous polarization. According to EL, the "fully" polarized state is among the degenerate ground states but the degeneracy cannot be lifted spontaneously if we do

not consider the magnetic moment of particles. Rojo[21] studied a two-component bosonic system which can be mapped into a "pseudo-spinor" Bose gas with $F = 1/2$ (without magnetic moments) and showed that the ground state is not polarized when the interaction is component-independent.

Within the interpretation that BEF is due to the magnetic moment, the *magnetic dipole interaction* between particles is implicitly involved. The dipole interaction is caused by the intrinsic field of magnetic moments which forms the internal magnetic field when magnetic moments are arranged parallel. The influence of magnetic dipole interactions on the properties of BEC has attracted considerable interest recently[22]. Although very weak, they can modify the ground state and the collective excitations of trapped condensates significantly[7, 22]. Our approach gives a new perspective for studying the effect of the dipole interactions on the boson gas. It is worth noting that dipole interactions can hardly result in a ferromagnetic state in a real Fermi gas, because the interaction is too weak to approach the Stoner threshold.

The intermediate area in Fig. 1 denotes the "pure" Bose-Einstein ferromagnetic state. This provides a direct way of detecting BEF experimentally. Once we have one experimental example pertaining to this regime, i.e., $c_2 > 0$ and the ground state is still ferromagnetic, the existence of BEF could be confirmed. The parameter $c_2 \propto (a_2 - a_0)/3$ can be estimated from experiments[5], where $a_2$ and $a_0$ are s-wave scattering lengths corresponding to the total spin two and zero channel, respectively. According to the above arguments,

$$(c_2)_c = \mu_0 \mathbf{m}^2, \qquad (14)$$

It is a rather small value. This makes the direct examination of BEF a difficult task.

Up to now, all of our discussions are devoted to chargeless bosons. One can expect that charged bosons exhibit more complex properties. For example, there would be a competition between the Bose-Einstein ferromagnetism and the Meissner effect, even though there is no external magnetic field applied. The latter tends to reduce or even to kill the magnetization. So, the nature of the ground state for charged spinor bosons is in our view still an open question. Relevant topics have been studied in triplet superconductors[23].

In conclusion, we have proposed a phenomenological model consistent with the prediction that magnetic bosons undergo a spontaneous magnetization together with Bose-Einstein condensation. We remark that this phenomenon deserves special attention due to two reasons: (i) It is an intrinsic property of spinor bosons and may be attributed to the magnetic moment of particles. (ii) The spontaneous magnetization is parasitic to the Bose-Einstein condensation, reflecting that the entropy of the Bose condensate is zero.

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[1] M.H. Anderson *et al.*, Science **269**, 198 (1995); K.B. Davis *et al.*, Phys. Rev. Lett. **75**, 3969 (1995); C.C. Bradley *et al.*, *ibid.* **75**, 1687 (1995).

[2] See for reviews, A.J. Leggett, Rev. Mod. Phys. **73**, 307 (2001) and F. Dalfovo *et al.*, *ibid.* **71**, 463 (1999)

[3] D.M. Stamper-Kurn *et al.*, Phys. Rev. Lett. **80**, 2027 (1998).

[4] J. Stenger *et al.*, Nature (London) **396**, 345 (1998).

[5] T.L. Ho, Phys. Rev. Lett. **81**, 742 (1998).

[6] T. Ohmi and K. Machida, J. Phys. Soc. Jpn. **67**, 1822 (1998).

[7] H. Pu, W. Zhang, and P. Meystre, Phys. Rev. Lett. **87**, 140405 (2001); W. Zhang *et al.*, *ibid.* **88**, 060401 (2002); K. Gross *et al.*, Phys. Rev. A **66**, 033603 (2002).

[8] E. Eisenberg and E.H. Lieb, Phys. Rev. Lett. **89**, 220403 (2002).

[9] K. Yamada, Prog. Theor. Phys. **67**, 443 (1982).

[10] M.V. Simkin and E.G.D. Cohen, Phys. Rev. A **59**, 1528 (1999).

[11] A. Caramico D'Auria, L. De Cesare, and I. Rabuffo, Physica A **225**, 363 (1996).

[12] A. Sütő, J. Phys. A **26**, 4689 (1993).

[13] V.L. Ginzburg and L.P. Pitaevskii, Sov. Phys. JETP **7**, 858 (1958).

[14] The Landau free energy in this form describes a spontaneous magnetization caused by other mechanisms. One can have $f_m$ in this form to study the interplay of the ferromagnetic and superfluid states. But that is not the purpose of this work.

[15] D.J. Craik, *Magnetism: principles and applications* (John Wiley & Sons, England, 1995).

[16] There are other solutions with higher free energies, including a trivial solution $|\Psi|^2 = 0$, $M = 0$ and a decoupled solution $|\Psi_1|^2 = |\Psi_{-1}|^2 = 0$, $|\Psi_0|^2 = \alpha/\beta$ with $M$ remaining arbitrary.

[17] D. Vollhardt and P. Wölfle, *The superfluid phases of Helium 3* (Taylor & Francis, London, 1990).

[18] Herein we suppose $\beta \gg g^2/a$. The free energy density corresponding to solution (II) can be written as $f_t^{II} = -\alpha|\Psi_1|^2 + (\beta - g^2/a)|\Psi_1|^4/2$. If $\beta < g^2/a$, higher-order expansions, e.g. $|\mathbf{\Psi}|^6$, were to be considered, the transition might be first order.

[19] T. Isoshima, K. Machida, and T. Ohmi, Phys. Rev. A **60**, 4857 (1999).

[20] L.P. Pitaevskii, Sov. Phys. JETP **13**, 451 (1961).

[21] A.G. Rojo, Phys. Rev. A **64**, 033608 (2001).

[22] See for example, K. Goral, K. Rzazewski, and T. Pfau, Phys. Rev. A **61**, 051601 (2000); J.-P. Martikainen, M. Mackie, and K.-A. Suominen, *ibid.* **64**, 037601 (2001); K. Goral, L. Santos, and M. Lewenstein, Phys. Rev. Lett. **88**, 170406 (2002); S. Giovanazzi, A. Görlitz, and T. Pfau, *ibid.* **89**, 130401 (2002).

[23] K. Scharnberg and R.A. Klemm, Phys. Rev. B **22**, 5233 (1980).